

Itinerant Antiferromagnetism of Correlated Lattice Fermions *

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Abstract

The problem of finding of the ferromagnetic and antiferromagnetic "symmetry broken" solutions of the correlated lattice fermion models beyond the mean-field approximation has been investigated. The calculation of the quasiparticle excitation spectra with damping for the single- and multi-orbital Hubbard model has been performed in the framework of the equation- of-motion method for two-time temperature Green's Functions within a non-perturbative approach. A unified scheme for the construction of Generalized Mean Fields (elastic scattering corrections) and self-energy (inelastic scattering) in terms of the Dyson equation has been generalized in order to include the presence of the "source fields". The damping of quasiparticles, which reflects the interaction of the single-particle and collective degrees of freedom has been calculated. The "symmetry broken" dynamical solutions of the Hubbard model, which correspond to various types of itinerant antiferromagnetism has been discussed. This approach complements previous studies and clarifies the nature of the concepts of itinerant antiferromagnetism and "spin-aligning field" of correlated lattice fermions.

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1 Introduction

The problem of the adequate description of strongly correlated lattice fermions has been studied intensively during the last decade, especially in the context of Heavy Fermions and High-T_c superconductivity [1] - [3]. The behaviour and the true nature of the electronic states and their quasiparticle dynamics is of central importance to the understanding of the magnetism in metals and the Mott-Hubbard metal-insulator transition in oxides, the heavy fermions in rare-earths compounds and the high-temperature superconductivity (HTSC) in cuprates. Recently there has been considerable interest in identifying the microscopic origin of these states [4]. Antiferromagnetic correlations may play an important role in the possible scenario of normal and superconducting behavior of these compounds. Some of the experimental and theoretical results show that antiferromagnetic spin fluctuations are really involved in the problem. This idea has stirred a great deal of discussion in recent times [5]. An appealing but phenomenological picture of HTSC, known as the nearly antiferromagnetic Fermi liquids (NAFL) approach, has been developed to explain many anomalous properties of cuprates [6]. This approach predicts the detailed phase diagram for cuprates [6] and present arguments which suggest that the physical origin of the pseudogap found in quasiparticle spectrum below the critical temperature is the formation of a precursor to a spin-density-wave-state. While the NAFL's scenario is appealing, it has apparently not yet been derived from fully microscopic consideration. The problem of the role of antiferromagnetic spin fluctuations for HTSC has recently been the subject of many papers(for a recent review see e.g. Ref. [7]). These investigations call for a better understanding of the nature of solutions (especially magnetic) to the Hubbard and related correlated models [8] - [11]. The microscopic theory of the itinerant ferromagnetism and antiferromagnetism [12], [13] of strongly correlated fermions on a lattice at finite temperatures is one of the important issues of recent efforts in the field [14] - [17]. In some papers the spin-density-wave (SDW) spectrum was only used without careful and complete analysis of the quasiparticle spectra of correlated lattice fermions. The aim of this paper is to investigate the intrinsic nature of the "symmetry broken" (ferro- and antiferromagnetic) solutions of the Hubbard model at finite temperatures from the many-body point of view. In the previous papers we set up the formalism and derived the equations for the quasiparticle spectra with damping within the single- and multi-orbital Hubbard model for the uniform paramagnetic case. In this paper we apply the formalism to consider the ferromagnetic and antiferromagnetic solutions. It is the purpose of this paper to explore more fully the notion of Generalized Mean Fields (GMF) [10] which may arise in the system of correlated lattice fermions to justify and understand the "nature" of the local staggered mean-fields which fix the antiferromagnetic ordering. The present work brings together the formulation of the itinerant antiferromagnetism of various papers. For this aim we rederive the SDW spectra by the Irreducible Green's Functions (IGF) method [18] taking into account the damping of quasiparticles. This alternative derivation has a close resemblance to that of the BCS theory of superconductivity for transition metals [19], [20] using the Nambu representation (c.f. [21]). This aspect of the theory is connected with the concept of broken symmetry, which is discussed in detail for the present case. The advantage of the Green's function method is the relative ease with which temperature effects may be calculated.

2 Itinerant Antiferromagnetism

The antiferromagnetic state is characterized by a spatially changing component of magnetisation which varies in such a way that the net magnetisation of the system is zero. The concept of antiferromagnetism of localized spins which is based on the Heisenberg model and the two-sublattice Neel ground state is relatively well founded contrary to the antiferromagnetism of delocalized or itinerant electrons. The itinerant-electron picture is the alternative conceptual picture for magnetism [22].

We now sketch the main ideas of the concept of itinerant antiferromagnetism. The simplified band model of an antiferromagnet has been formulated by Slater [23] within the single-particle Hartree-Fock (H-F) approximation. In this approach he used the "exchange repulsion" to keep electrons with parallel spins away from each other and to lower the Coulomb interaction energy. Some authors consider it as a prototype of the Hubbard model. However the exchange repulsion was taken proportional to the number of electrons with the same spins only and the energy gap between two subbands was proportional to the difference of electrons with up and down spins. In the antiferromagnetic many-body problem there is an additional "symmetry broken" aspect. For an antiferromagnet, contrary to ferromagnet, the one-electron H-F potential can violate the translational crystal symmetry. The period of the antiferromagnetic spin structure L is greater than the lattice constant a . To introduce the two-sublattice picture for itinerant model one should assume that $L = 2a$ and that the spins of outer electrons on neighboring atoms are antiparallel to each other. In other words, the alternating (H-F) potential $v_{i\sigma} = -\sigma v \exp(iQR_i)$ where $Q = (\pi/2, \pi/2, \pi/2)$ corresponds to a two-sublattice AFM structure. To justify an antiferromagnetic ordering with alternating up and down spin structure we must admit that in effect two different charge distributions will arise concentrated on atoms of sublattices A and B. This picture accounts well for quasi-localized magnetic behavior.

The earlier theories of itinerant antiferromagnetism were proposed by des Cloizeaux [24] and especially Overhauser [25] (in the context of the investigation of the ground state of nuclear matter). Then Overhauser [26] has applied this approach for the explanation of the anomalous properties of dilute $Cu - Mn$ alloys, has suggested an antiferromagnetic mechanism that requires neither two-body interactions between paramagnetic solute spins, nor a sublattice structure (c.f. [27]). Such a mechanism may be recognized by considering a new type excited state of the conduction electron gas. He invented the static SDW which allow the total charge density of the gas to remain spatially uniform. Overhauser [25] - [29] suggested that the H-F ground state of a three dimensional electron gas is not necessarily a Slater determinant of plane waves. Alternative sets of one-particle states can lead to a lower ground-state energy. Among these alternatives to the plane-wave state are the SDW and CDW ground states for which the one-electron Hamiltonians have the form

$$H = (p^2/2m) - G(\sigma_x \cos Qz + \sigma_y \sin Qz) \quad (1)$$

(spiral SDW; $Q = 2k_F z$)

and

$$H = (p^2/2m) - 2G \cos(Qr) \quad (2)$$

(CDW; $Q = 2k_F z$)

The periodic potentials in the above expressions lead to a corresponding variation in the electronic spin and charge densities, accompanied by a compensating variation of the background.

The effect of Coulomb interaction on the magnetic properties of the electron gas in Overhauser's approach renders the paramagnetic plane-wave state of the free-electron-gas model unstable within the H-F approximation. The long-range components of the Coulomb interaction are most important in creating this instability [29]. It was demonstrated [28] that a nonuniform static SDW is lower in energy than the uniform (paramagnetic state) in the Coulomb gas within the H-F approximation for certain electron density.

The H-F is the simplest approximation but neglects the important dynamical part. To include the dynamics one should take into consideration the correlation effects. The role of correlation corrections which tend to suppress the SDW state as well as the role of shielding and screening were not fully clarified [30]. Overhauser remarked that SDW ground states do not occur for δ -function interactions, whatever their strength. This question was investigated further in Ref. [31]. An instability of the paramagnetic Hartree-Fock state against a state with different orbitals for different spins was interpreted as a magnetic phase transition.

It is important to note that in the Slater's and des Cloiseaux's models an electron moving in a crystal does not change its spin. In these models the main processes are related with the pairing of electrons having the same spins, one from each of the two sublattices. In the Overhauser's approach to itinerant antiferromagnetism the combination of the electronic states with different spins (with pairing of the opposite spins) is used to describe the SDW state with period Q . The first approach is obviously valid only in the simple commensurate two-sublattice case and the latter is applicable to the more general case of an incommensurate spiral spin state. The general SDW state has the form

$$\Psi_{p\sigma} = \chi_{p\sigma} \cos(\theta_p/2) + \chi_{p+Q-\sigma} \sin(\theta_p/2) \quad (3)$$

The average spin for helical or spiral spin arrangement changes its direction in the (x-y) plane. For the spiral SDW states a spatial variation of magnetisation corresponds to $\vec{Q} = (\frac{\pi}{a})(1, 1)$. The antiferromagnetic phase of chromium [32], [33] and its alloys has been satisfactorily explained in terms of the SDW within a two-band model [34]. It is essential to note that chromium becomes antiferromagnetic in a unique manner. The antiferromagnetism is established in a more subtle way from the spins of the itinerant electrons than the magnetism of collective band electrons in metals like iron and nickel. The essential feature of chromium which makes possible the formation of the SDW is the existence of "nested" portions of the Fermi surface [33]. The formation of bound electron-hole pairs takes place between particles of opposite spins; the condensed state exhibits the SDW.

The recent attempt to describe an antiferromagnetic insulator at $T = 0$ using a one-electron approach was made in Ref. [35]. To do this, the authors proposed to overcome the inadequacies of standard local-spin-density theory by adding a spin-dependent magnetic pseudopotential to Kohn-Sham equations.

For the Hubbard model [36] the qualitative phase diagram was calculated by Penn [37]. Unfortunately, although his work gives a clear physical picture, it does not emphasize the lattice character of the tight-binding or Wannier fermions as well as the essence of the anomalous spin-flip averages. The Hubbard model is a simplified but workable model for the correlated lattice fermions and the applicability of the SDW Overhauser concept to highly correlated tight binding electrons on a lattice deserves a careful analysis within this model. In earlier papers [38] - [41] the single- and multi-orbital Hubbard model has been investigated with respect to antiferromagnetic solutions in the mean-field approximation mainly.

3 Hubbard Model

The Hubbard model has been widely recognised as a workable model for a study of the correlated itinerant electron systems. For the sake of completeness we shall discuss the single-orbital and multi-orbital cases separately.

3.1 MULTI-ORBITAL HUBBARD MODEL

To demonstrate the advantage of our approach we shall consider the quasiparticle spectrum of the lattice fermions for degenerate band model. Let us start with the second quantized form of the Hamiltonian taking the set of the Wannier functions $[\phi_\lambda(r - R_i)]$. Here λ is the band index ($\lambda = 1, 2, \dots, 5$).

$$H = \sum_{ij\mu\nu\sigma} t_{ij}^{\mu\nu} a_{i\mu\sigma}^+ a_{j\nu\sigma} + \frac{1}{2} \sum_{ij,mn} \sum_{\alpha\beta\gamma\delta\sigma\sigma'} < i\alpha, j\beta | W | m\gamma, n\delta > a_{i\alpha\sigma}^+ a_{j\beta\sigma'}^+ a_{m\gamma\sigma'} a_{n\delta\sigma} \quad (4)$$

For a degenerate d-band the second quantized form of the total Hamiltonian in the Wannier-function representation reduces to the following model Hamiltonian

$$H = H_1 + H_2 + H_3 \quad (5)$$

The kinetic energy operator is given by

$$H_1 = \sum_{ij} \sum_{\mu\nu\sigma} t_{ij}^{\mu\nu} a_{i\mu\sigma}^+ a_{j\nu\sigma} \quad (6)$$

The term H_2 describes one-centre Coulomb interactions

$$\begin{aligned} H_2 = & \frac{1}{2} \sum_{i\mu\sigma} U_{\mu\mu} n_{i\mu\sigma} n_{i\mu-\sigma} + \frac{1}{2} \sum_{i\mu\nu} \sum_{\sigma\sigma'} V_{\mu\nu} n_{i\mu\sigma} n_{i\nu\sigma'} (1 - \delta_{\mu\nu}) - \\ & \frac{1}{2} \sum_{i\mu\nu\sigma} I_{\mu\nu} n_{i\mu\sigma} n_{i\nu\sigma} (1 - \delta_{\mu\nu}) + \frac{1}{2} \sum_{i\mu\nu\sigma} I_{\mu\nu} a_{i\mu\sigma}^+ a_{i\mu-\sigma}^+ a_{i\nu-\sigma} a_{i\nu\sigma} (1 - \delta_{\mu\nu}) - \\ & \frac{1}{2} \sum_{i\mu\nu\sigma} I_{\mu\nu} a_{i\mu\sigma}^+ a_{i\mu-\sigma} a_{i\nu-\sigma}^+ a_{i\nu\sigma} (1 - \delta_{\mu\nu}) \end{aligned} \quad (7)$$

In addition to the intrasite intraorbital interaction $U_{\mu\mu}$ which is the only interaction present in the single-orbital Hubbard model, this term contains three more kinds of interorbital interactions.

The last term H_3 describes the direct intersite exchange interaction

$$H_3 = -\frac{1}{2} \sum_{ij\mu} \sum_{\sigma\sigma'} J_{ij}^{\mu\mu} a_{i\mu\sigma}^+ a_{i\mu-\sigma'} a_{j\mu\sigma'}^+ a_{j\mu\sigma} \quad (8)$$

The definition of various integrals in H is obvious. It is reasonable to assume that:

$$U_{\mu\mu} = U; \quad V_{\mu\nu} = V; \quad I_{\mu\nu} = I; \quad J_{ij}^{\mu\mu} = J_{ij}. \quad (9)$$

This Hamiltonian differ slightly from the analogous Hamiltonian of Ref. [40] where the only intrasite interaction terms of the second-quantized Hamiltonian of the d -band were taken into consideration.

3.2 SINGLE-ORBITAL HUBBARD MODEL

The model Hamiltonian which is usually referred to as Hubbard Hamiltonian [36]

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \quad (10)$$

includes the intraatomic Coulomb repulsion U and the one-electron hopping energy t_{ij} . The electron correlation forces electrons to localize in the atomic orbitals, which are modelled here by the complete and orthogonal set of the Wannier wave functions $[\phi(\vec{r} - \vec{R}_j)]$. (The Wannier representation, which is a unitary transformation of the Bloch representation is an important background of the Hubbard model. It is well known that in one-dimension the Wannier functions decrease exponentially but less is known about two- and three-dimensional cases.) On the other hand, the kinetic energy is reduced when electrons are delocalized. The main difficulty of the right solution of the Hubbard model is the necessity of taking into account both these effects simultaneously. Thus, the Hamiltonian (10) is specified by two parameters: U and effective electron bandwidth

$$\Delta = (N^{-1} \sum_{ij} |t_{ij}|^2)^{1/2}.$$

The important third "player" is the Pauli principle, which has a long-range character, contrary to the local Coulomb repulsion and nearest-neighbour hopping.

The band energy of Bloch electrons $\epsilon(\vec{k})$ is defined as follows

$$t_{ij} = N^{-1} \sum_{\vec{k}} \epsilon(\vec{k}) \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)],$$

where N is the number of the lattice sites. It is convenient to count the energy from the center of gravity of the band, i.e. $t_{ii} = \sum_k \epsilon(k) = 0$. The effective electron bandwidth Δ and Coulomb intrasite integral U define completely the different regimes in 3 dimension depending on parameter $\gamma = \Delta/U$. It is usually a rather difficult task to find interpolating solution for the dynamical properties of the Hubbard model. We evidently have to improve the early Hubbard's theory taking account of the variety of possible regimes for the model depending on electronic density, temperature and values of γ . It was the purpose of the papers [3], [10] to find the electronic quasiparticle spectra in a wide range of the temperature and the parameters of the model and to account explicitly for the contribution of damping of the electronic states when calculating the various characteristics of the model. In the past years many theoretical papers have been published, in which the approximative dynamical solution of the models (5) and (10) has been investigated by means of various advanced methods of many-body theory. Despite the considerable contributions to the development of the many-body theory and to our better understanding of the physics of the correlated electron systems, the fully consistent dynamical analytical solution of the Hubbard model is still lacking. To solve this problem with a reasonably accuracy and to describe correctly an interpolating solution one need a more sophisticated approach than the usual procedures which have been developed for description of the interacting electron-gas- problem.

4 Irreducible Green's Functions Method

Recent theoretical investigations of strongly correlated electron systems have brought forward a significant variety of approaches. To describe from first principles of the condensed matter

theory and statistical mechanics the physical properties of strongly correlated systems we need to develop a systematic theory of quasiparticle spectra.

In this paper we will use the approach which allows one to describe completely the quasi-particle spectra with damping in a very natural way. This approach has been suggested to be essential for various many-body systems and we believe that it bears the real physics of strongly correlated electron systems [10], [18]. The essence of our consideration of the dynamical properties of many-body system with strong interaction is related closely with the field theoretical approach and use the advantage of the Green's functions language and the Dyson equation. It is possible to say that our method tend to emphasize the fundamental and central role of the Dyson equation for the single-particle dynamics of the many-body systems at finite temperatures.

In this Section, we will discuss briefly this novel nonperturbative approach for the description of the many-body dynamics of strongly correlated systems. A number of other approaches has been proposed and our approach is in many respect additional and incorporates the logic of development of the many-body techniques. The considerable progress in studying the spectra of elementary excitations and thermodynamic properties of many-body systems has been for most part due to the development of the temperature dependent Green's Functions methods. We have developed a helpful reformulation of the two-time GFs method which is especially adjusted [3] for the correlated fermion systems on a lattice. The very important concept of the whole method are the **Generalized Mean Fields**. These GMFs have a complicated structure for the strongly correlated case and do not reduce to the functional of the mean densities of the electrons, when we calculate excitations spectra at finite temperatures. To clarify the foregoing, let us consider the retarded GF of the form

$$G^r = \langle\langle A(t), B(t') \rangle\rangle = -i\theta(t - t') \langle [A(t)B(t')]_\eta \rangle, \eta = \pm 1. \quad (11)$$

As an introduction of the concept of IGFs let us describe the main ideas of this approach in a symbolic form. To calculate the retarded GF $G(t - t')$ let us write down the equation of motion for it:

$$\omega G(\omega) = \langle [A, A^+]_\eta \rangle + \langle\langle [A, H]_- | A^+ \rangle\rangle_\omega. \quad (12)$$

The essence of the method is as follows [18]. It is based on the notion of the "*IRREDUCIBLE*" parts of GFs (or the irreducible parts of the operators, out of which the GF is constructed) in term of which it is possible, without recourse to a truncation of the hierarchy of equations for the GFs, to write down the exact Dyson equation and to obtain an exact analytical representation for the self-energy operator. By definition we introduce the irreducible part (**ir**) of the GF

$${}^{ir} \langle\langle [A, H]_- | A^+ \rangle\rangle = \langle\langle [A, H]_- - zA | A^+ \rangle\rangle. \quad (13)$$

The unknown constant z is defined by the condition (or constraint)

$$\langle [A, H]_-^{ir}, A^+ \rangle_\eta = 0 \quad (14)$$

From the condition (14) one can find:

$$z = \frac{\langle [A, H]_-, A^+ \rangle_\eta}{\langle [A, A^+]_\eta \rangle} = \frac{M_1}{M_0} \quad (15)$$

Here M_0 and M_1 are the zeroth and first order moments of the spectral density. Therefore, irreducible GF are defined so that they cannot be reduced to the lower-order ones by any kind

of decoupling. It is worthy to note that the irreducible correlation functions are well known in statistical mechanics. In the diagrammatic approach the irreducible vertices are defined as the graphs that do not contain inner parts connected by the G^0 -line. With the aid of the definition (13) these concepts are translated into the language of retarded and advanced GFs. This procedure extract all relevant (for the problem under consideration) mean field contributions and puts them into the generalized mean-field GF, which here are defined as

$$G^0(\omega) = \frac{<[A, A^+]_\eta>}{(\omega - z)}. \quad (16)$$

To calculate the IGF $^{ir} << [A, H]_-(t), A^+(t') >>$ in (12), we have to write the equation of motion after differentiation with respect to the second time variable t' . The condition (14) removes the inhomogeneous term from this equation and is a very crucial point of the whole approach. If one introduces an irreducible part for the right-hand side operator as discussed above for the “left” operator, the equation of motion (12) can be exactly rewritten in the following form

$$G = G^0 + G^0 P G^0. \quad (17)$$

The scattering operator P is given by

$$P = (M_0)^{-1} \quad ^{ir} << [A, H]_- | [A^+, H]_- >>^{ir} (M_0)^{-1}. \quad (18)$$

The structure of the equation (17) enables us to determine the self-energy operator M , in complete analogy with the diagram technique

$$P = M + M G^0 P. \quad (19)$$

From the definition (19) it follows that the self-energy operator M is defined as a proper (in diagrammatic language “connected”) part of the scattering operator $M = (P)^p$. As a result, we obtain the exact Dyson equation for the thermodynamic two-time Green’s Functions:

$$G = G^0 + G^0 M G, \quad (20)$$

which has a well known formal solution of the form

$$G = [(G^0)^{-1} - M]^{-1} \quad (21)$$

Thus, by introducing irreducible parts of GF (or the irreducible parts of the operators, out of which the GF is constructed) the equation of motion (12) for the GF can be exactly (but using constraint (14)) transformed into Dyson equation for the two-time thermal GF. This is very remarkable result, which deserves underlining, because of the traditional form of the GF method did not include this point. The projection operator technique has essentially the same philosophy, but with using the constraint (14) in our approach we emphasize the fundamental and central role of the Dyson equation for the calculation of the single-particle properties of the many-body systems. It is important to note, that for the retarded and advanced GFs the notion of the proper part is symbolic in nature [18]. However, because of the identical form of the equations for the GFs for all three types (advanced, retarded and causal), we can convert in each stage of calculations to causal GFs and, thereby, confirm the substantiated nature of definition (19)! We therefore should speak of an analogue of the Dyson equation. Hereafter we

will drop this stipulation, since it will not cause any misunderstanding. It should be emphasized that the scheme presented above give just an general idea of the IGF method. The specific method of introducing IGFs depends on the form of operator A , the type of the Hamiltonian and the conditions of the problem. The general philosophy of the IGF method lies in the separation and identification of elastic scattering effects and inelastic ones. This last point is quite often underestimated and both effects are mixed. However, as far as the right definition of quasiparticle damping is concerned, the separation of elastic and inelastic scattering processes is believed to be crucially important for the many-body systems with complicated spectra and strong interaction. Recently it was emphasized especially that the anomalous damping of electrons (or holes) distinguishes cuprate superconductors from ordinary metals. From a technical point of view the elastic (GMF) renormalizations can exhibit a quite non-trivial structure. To obtain this structure correctly, one must construct the full GF from the complete algebra of the relevant operators and develop a special projection procedure for higher-order GF in accordance with a given algebra. It is necessary to emphasize that that there is an intimate connection between the adequate introduction of mean fields and internal symmetries of the Hamiltonian.

5 Symmetry Broken Solutions

In many-body interacting systems, the symmetry is important in classifying of the different phases and in understanding of the phase transitions between them [42] - [48]. According to Bogolubov [42] (c.f. [47]) in each condensed phase, in addition to the normal process, there is an anomalous process (or processes) which can take place because of the long-range internal field, with a corresponding propagator. The anomalous propagators for interacting many-fermion system corresponding to the ferromagnetic (FM) and antiferromagnetic (AFM) long-range ordering are given by

$$\begin{aligned} FM : G_{fm} &\sim \langle \langle a_{k\sigma}; a_{k-\sigma}^+ \rangle \rangle \\ AFM : G_{afm} &\sim \langle \langle a_{k+Q\sigma}; a_{k+Q'\sigma'}^+ \rangle \rangle \end{aligned} \quad (22)$$

In the SDW case, a particle picks up momentum $Q - Q'$ from scattering against the periodic structure of the spiral (nonuniform) internal field, and has its spin changed from σ to σ' by the spin-aligning character of the internal field. The Long-Range-Order (LRO) parameters are:

$$\begin{aligned} FM : m &= 1/N \sum_{k\sigma} \langle a_{k\sigma}^+ a_{k-\sigma} \rangle \\ AFM : M_Q &= \sum_{k\sigma} \langle a_{k\sigma}^+ a_{k+Q-\sigma} \rangle \end{aligned} \quad (23)$$

It is important to note that the long-range order parameters are functions of the internal field, which is itself a function of the order parameter. There is a more mathematical way of formulating this assertion. According to the paper [14], the notion "symmetry breaking" means that the state fails to have the symmetry that the Hamiltonian has. True broken symmetry can arise only if there are infinitesimal "source fields" present. Indeed, for the rotationally and translationally invariant Hamiltonian the suitable source terms should be added:

$$\begin{aligned} FM : \varepsilon \mu_B H_x \sum_{k\sigma} a_{k\sigma}^+ a_{k-\sigma} \\ AFM : \varepsilon \mu_B H \sum_{kQ} a_{k\sigma}^+ a_{k+Q-\sigma} \end{aligned} \quad (24)$$

where $\varepsilon \rightarrow 0$ is to be taken at the end of calculations.

Broken symmetry solutions of the Overhauser type (3) imply that the vector Q is a measure of the inhomogeneity or breaking of translational symmetry. It is interesting to note the remark of paper [46](c.f. [48]) about antiferromagnetism, for which "a staggered magnetic field plays the role of symmetry-breaking field. No mechanism can generate a real staggered magnetic field in an antiferromagnetic material". The Hubbard model is a very interesting tool for the analyzing this concept [41] - [51].

Penn [37] shown that antiferromagnetic state and more complicated states (e.g. ferrimagnetic) can be made eigenfunctions of the self-consistent field equations within an "extended" mean-field approach, assuming that the "anomalous" averages $\langle a_{i\sigma}^+ a_{i-\sigma} \rangle$ determine the behavior of the system on the same footing as the "normal" density of quasiparticles $\langle a_{i\sigma}^+ a_{i\sigma} \rangle$. It is clear, however, that these "spin-flip" terms break the rotational symmetry of the Hubbard Hamiltonian. For the single- band Hubbard Hamiltonian the averaging $\langle a_{i-\sigma}^+ a_{i,\sigma} \rangle = 0$ because of the rotational symmetry of the Hubbard model. The inclusion of the "anomalous" averages lead to the unresricted H-F approximation. The rigorous definition of the unrestricted Hartree-Fock approximation (UHFA) has been done recently in Ref. [14]. This approximation has been applied also for the single-band Hubbard model (10) for the calculation of the density of states. The following definition of UHFA has been used:

$$n_{i-\sigma} a_{i\sigma} = \langle n_{i-\sigma} \rangle a_{i\sigma} - \langle a_{i-\sigma}^+ a_{i\sigma} \rangle a_{i-\sigma} \quad (25)$$

Thus, in addition to the standard H-F term, the new, the so-called "spin-flip" terms, are retained. This example clearly show that the nature of the mean-fields follows from the essentials of the problem and should be defined in a proper way. So, one needs a properly defined effective Hamiltonian H_{eff} . We shall analyze below in detail the proper definition of the irreducible GFs which include the "spin-flip" terms. For the single-orbital Hubbard model this definition should be modified in the following way:

$$\begin{aligned} ir \langle\langle a_{k+p\sigma} a_{p+q-\sigma}^+ a_{q-\sigma} | a_{k\sigma}^+ \rangle\rangle_{\omega} = & \langle\langle a_{k+p\sigma} a_{p+q-\sigma}^+ a_{q-\sigma} | a_{k\sigma}^+ \rangle\rangle_{\omega} - \\ & \delta_{p,0} \langle n_{q-\sigma} \rangle G_{k\sigma} - \langle a_{k+p\sigma} a_{p+q-\sigma}^+ \rangle \langle\langle a_{q-\sigma} | a_{k\sigma}^+ \rangle\rangle_{\omega} \end{aligned} \quad (26)$$

From this definition it follows that such way of introduction of the IGF broadens the initial algebra of the operators and the initial set of the GFs. This means that "actual" algebra of the operators must include the spin-flip terms at the beginning, namely: $(a_{i\sigma}, a_{i\sigma}^+, n_{i\sigma}, a_{i\sigma}^+ a_{i-\sigma})$. The corresponding initial GF will have the form

$$\begin{pmatrix} \langle\langle a_{i\sigma} | a_{j\sigma}^+ \rangle\rangle & \langle\langle a_{i\sigma} | a_{j-\sigma}^+ \rangle\rangle \\ \langle\langle a_{i-\sigma} | a_{j\sigma}^+ \rangle\rangle & \langle\langle a_{i-\sigma} | a_{j-\sigma}^+ \rangle\rangle \end{pmatrix}$$

With this definition we introduce the so-called anomalous (off-diagonal) GFs which fix the relevant vacuum and select the proper symmetry broken solutions. In fact, this approximation has been investigated earlier by Kishore and Joshi [50]. They clearly pointed out that they assumed that the system is magnetized in the x direction instead of the conventional z axis. The detailed investigation and classification of the magnetic and non-magnetic symmetry broken solutions of the three-band extended Hubbard model for CuO_2 planes of high- T_c superconductors was made in Ref. [51] within the mean-field approximation.

6 Dynamical Properties

In many-body interacting systems the quasiparticle dynamics can be quite non-trivial. Here the problem of the adequate description of the many-body dynamics of the multi-orbital Hubbard model will be discussed in the framework of the equation-of-motion approach for two-time thermodynamic Green's Functions. Our main motivation was the intention to formulate a consistent theory of dynamical properties of the Hubbard model taking into account the symmetry broken (magnetic) solutions.

This formulation gives us an opportunity to emphasize some important issues about the relevant dynamical solutions of the strongly correlated models of fermions on a lattice and to formulate in a more sharp form the ideas of the method of the Irreducible Green's Functions (IGF) [18]. This IGF method allows one to describe the quasiparticle spectra with damping of the strongly correlated electron systems in a very general and natural way and to construct the relevant dynamical solution in a self-consistent way on the level of the Dyson equation without decoupling the chain of the equation of motion for the GFs.

The interplay and the competition of the kinetic energy and potential energy affects substantially the electronic spectrum. The renormalized electron energies are temperature dependent and the electronic states have finite life times. These effects are most suitably accounted for by the Green's functions method. We shall use the (IGF) method of Section 4. To give a more instructive discussion let us consider the single-particle GF of lattice fermions, which is defined as

$$G_{\sigma\sigma'}^{\mu\nu}(ij; t - t') = \langle\langle a_{i\mu\sigma}(t), a_{j\nu\sigma'}^+(t') \rangle\rangle = -i\theta(t - t') \langle [a_{i\mu\sigma}(t), a_{j\nu\sigma'}^+(t')]_+ \rangle = \\ 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t) G_{\sigma\sigma'}^{\mu\nu}(ij; \omega) \quad (27)$$

Actually, this GF is a matrix (10x10) in the joint tensor product vector space of spin and orbital momentum. The diagonal elements of this matrix GF are normal propagators, while the off-diagonal elements are anomalous. The equation of motion for the Fourier transform of the GF has the form

$$\sum_{m\alpha} A^{\mu\alpha}(im) G_{\sigma\sigma'}^{\alpha\nu}(mj; \omega) = \delta_{ij} \delta_{\mu\nu} \delta_{\sigma\sigma'} + \sum_{m\alpha} [B_1^{\mu\alpha}(im) \langle\langle a_{m\mu\sigma} n_{m\alpha\sigma} | a_{j\nu\sigma'}^+ \rangle\rangle + \\ B_2^{\mu\alpha}(im) \langle\langle a_{m\mu\sigma} n_{m\alpha-\sigma} | a_{j\nu\sigma'}^+ \rangle\rangle + \\ B_3^{\mu\alpha}(im) (\langle\langle a_{i\mu\sigma} n_{m\mu\sigma} | a_{j\nu\sigma'}^+ \rangle\rangle + \langle\langle a_{i\mu-\sigma} a_{m\mu-\sigma}^+ a_{m\mu\sigma} | a_{j\nu\sigma'}^+ \rangle\rangle)] \quad (28)$$

Here we have introduced the notations

$$A^{\mu\alpha}(im) = \omega \delta_{mi} \delta_{\mu\alpha} - t_{im}^{\mu\alpha}; \quad B_1^{\mu\alpha}(im) = (V - I) \delta_{im} (1 - \delta_{\mu\alpha}); \quad (29) \\ B_2^{\mu\alpha} = [U \delta_{\mu\alpha} + V (1 - \delta_{\mu\alpha})] \delta_{im}; \quad B_3^{\mu\alpha}(im) = J_{im} (1 - \delta_{im}) \delta_{\mu\alpha}$$

Let us introduce, by definition, an "irreducible" GF in the following way

$$(^{ir} \langle\langle a_{i\beta\sigma} a_{m\alpha\sigma_1}^+ a_{m\alpha\sigma_1} | a_{j\nu\sigma'}^+ \rangle\rangle) = \langle\langle a_{i\beta\sigma} a_{m\alpha\sigma_1}^+ a_{m\alpha\sigma_1} | a_{j\nu\sigma'}^+ \rangle\rangle \quad (30) \\ - \langle n_{m\alpha\sigma_1} \rangle \delta_{mi} \langle\langle a_{i\beta\sigma} | a_{j\nu\sigma'}^+ \rangle\rangle - \langle a_{i\beta\sigma} a_{m\alpha\sigma_1}^+ \rangle \langle\langle a_{m\alpha\sigma_1} | a_{j\nu\sigma'}^+ \rangle\rangle$$

According to (14), the following constraint should be valid

$$\langle [(a_{i\beta\sigma} n_{m\alpha\sigma_1})^{(ir)}, a_{j\nu\sigma'}^+]_+ \rangle = 0 \quad (31)$$

Substituting (30) in (28) we obtain the following equation of motion in the matrix (in spin space) form

$$\sum_{m\alpha} F^{\mu\alpha}(im) G^{\alpha\nu}(mj; \omega) = 1 + \sum_{m\alpha} [L_1^{\mu\alpha}(il) D_1^{\mu\alpha\nu}(mj) + L_2^{\mu\alpha}(im) D_2^{\mu\alpha\nu}(mj) + L_3^{\mu\alpha}(im) (R_1^{\alpha\nu}(im, j) + R_2^{\alpha\nu}(im, j))] \quad (32)$$

where

$$\begin{aligned} F^{\mu\alpha}(im) &= \begin{pmatrix} E_{11}^{\mu\alpha}(im) & E_{12}^{\mu\alpha}(im) \\ E_{21}^{\mu\alpha}(im) & E_{22}^{\mu\alpha}(im) \end{pmatrix}; \quad 1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \delta_{\mu\nu} \delta_{ij} \\ L_1^{\mu\alpha}(im) &= \begin{pmatrix} B_1^{\mu\alpha}(im) & B_2^{\mu\alpha} \\ 0 & 0 \end{pmatrix}; \quad L_2^{\mu\alpha}(im) = \begin{pmatrix} 0 & 0 \\ B_1^{\mu\alpha}(im) & B_2^{\mu\alpha}(il) \end{pmatrix}; \\ L_3^{\mu\alpha}(im) &= \begin{pmatrix} B_3^{\mu\alpha}(im) & 0 \\ 0 & B_3^{\mu\alpha}(im) \end{pmatrix} \end{aligned} \quad (33)$$

and

$$\begin{aligned} E_{11}^{\mu\alpha}(im) &= A^{\mu\alpha}(im) - B_1^{\mu\alpha}(im) \langle a_{m\mu\uparrow} a_{m\alpha\uparrow}^+ \rangle - \sum_{\beta} (B_1^{\mu\beta}(im) \langle n_{m\alpha\uparrow} \rangle \delta_{\mu\beta} - B_2^{\mu\beta}(im) \langle n_{i\alpha\downarrow} \rangle \delta_{\mu\beta}) - \\ &B_3^{\mu\alpha}(im) (\langle a_{i\alpha\uparrow} a_{m\alpha\uparrow}^+ \rangle + \langle a_{i\alpha\downarrow} a_{m\alpha\downarrow}^+ \rangle) - \sum_l B_3^{\mu\alpha}(ml) \langle n_{l\alpha\uparrow} \rangle; \\ E_{12}^{\mu\alpha} &= -B_2^{\mu\alpha} \langle a_{m\mu\uparrow} a_{m\alpha\downarrow}^+ \rangle - \sum_l B_3^{\mu\alpha} \langle a_{l\alpha\downarrow}^+ a_{l\alpha\uparrow} \rangle \delta_{im} \end{aligned} \quad (34) \quad (35)$$

and similar expressions for E_{21} and E_{22} with reversed spin indices. The higher-order GF have the form

$$\begin{aligned} D_1 &= \begin{pmatrix} ((ir) \langle \langle a_{m\mu\uparrow} n_{m\alpha\uparrow} | a_{j\nu\uparrow}^+ \rangle \rangle) & ((ir) \langle \langle a_{m\mu\uparrow} n_{m\mu\uparrow} | a_{j\nu\downarrow}^+ \rangle \rangle) \\ ((ir) \langle \langle a_{m\mu\uparrow} n_{m\alpha\downarrow} | a_{j\nu\uparrow}^+ \rangle \rangle) & ((ir) \langle \langle a_{m\mu\uparrow} n_{m\alpha\downarrow} | a_{j\nu\downarrow}^+ \rangle \rangle) \end{pmatrix} \\ D_2 &= \begin{pmatrix} ((ir) \langle \langle a_{i\alpha\uparrow} n_{m\alpha\uparrow} | a_{j\nu\uparrow}^+ \rangle \rangle) & ((ir) \langle \langle a_{i\alpha\uparrow} n_{m\alpha\uparrow} | a_{j\nu\downarrow}^+ \rangle \rangle) \\ ((ir) \langle \langle a_{i\alpha\downarrow} n_{m\alpha\downarrow} | a_{j\nu\uparrow}^+ \rangle \rangle) & ((ir) \langle \langle a_{i\alpha\downarrow} n_{m\alpha\downarrow} | a_{j\nu\downarrow}^+ \rangle \rangle) \end{pmatrix} \end{aligned} \quad (36)$$

and R has the following structure

$$R = \begin{pmatrix} ((ir) \langle \langle a_{m\mu\uparrow} a_{m\alpha\uparrow}^+ a_{m\alpha\uparrow} | a_{n\nu\uparrow}^+ \rangle \rangle) & ((ir) \langle \langle a_{m\mu\uparrow} a_{m\alpha\uparrow}^+ a_{m\alpha\uparrow} | a_{n\nu\downarrow}^+ \rangle \rangle) \\ ((ir) \langle \langle a_{m\mu\uparrow} a_{m\alpha\downarrow}^+ a_{m\alpha\downarrow} | a_{n\nu\uparrow}^+ \rangle \rangle) & ((ir) \langle \langle a_{m\mu\uparrow} a_{m\alpha\downarrow}^+ a_{m\alpha\downarrow} | a_{n\nu\downarrow}^+ \rangle \rangle) \end{pmatrix}$$

To calculate the higher-order GF D_1 , D_2 , R_1 and R_2 , we will differentiate the r.h.s. of it with respect to the second-time variable (t'). Combining both (the first- and second-time differentiated) equations of motion we get the "exact" (no approximation have been made till now) "scattering" equation

$$G^{\mu\nu}(ij; \omega) = G_0^{\mu\nu}(ij; \omega) + \sum_{mn\alpha\beta} G_0^{\mu\alpha}(im; \omega) P^{\alpha\beta}(mn; \omega) G_0^{\beta\nu}(nj; \omega) \quad (37)$$

Here we have introduced the generalized mean-field (GMF) GF G_0 according to the following definition

$$\sum_{m\alpha} F^{\mu\alpha}(im) G_0^{\alpha\nu}(mj; \omega) = \delta_{ij} \delta_{\mu\nu} \quad (38)$$

The scattering operator P has the form

$$P^{\mu\alpha}(mn; \omega) = \begin{pmatrix} P_{11}^{\mu\alpha}(mn; \omega) & P_{12}^{\mu\alpha}(mn; \omega) \\ P_{21}^{\mu\alpha}(mn; \omega) & P_{22}^{\mu\alpha}(mn; \omega) \end{pmatrix}; \quad (39)$$

Let us write down explicitly the first matrix element

$$\begin{aligned} P_{11}^{\alpha\beta}(mn; \omega) = & \sum_{ij\mu\nu} [B_1^{\mu\alpha}(im) \langle \langle a_{m\mu\uparrow} n_{m\alpha\uparrow} | a_{n\nu\uparrow}^+ n_{n\beta\uparrow} \rangle \rangle^{(ir)} B_1^{\mu\beta}(nj) + \\ & B_1^{\mu\alpha}(im) \langle \langle a_{m\mu\uparrow} n_{m\alpha\uparrow} | a_{n\nu\uparrow}^+ n_{n\beta\downarrow} \rangle \rangle^{(ir)} B_2^{\beta\nu}(nj) + \\ & B_2^{\mu\alpha}(im) \langle \langle a_{m\mu\uparrow} n_{m\alpha\downarrow} | a_{n\nu\uparrow}^+ n_{n\beta\uparrow} \rangle \rangle^{(ir)} B_1^{\beta\nu}(nj) + \\ & B_2^{\mu\alpha}(im) \langle \langle a_{m\mu\uparrow} n_{m\alpha\downarrow} | a_{n\nu\uparrow}^+ n_{n\beta\downarrow} \rangle \rangle^{(ir)} B_2^{\beta\nu}(nj)] \end{aligned} \quad (40)$$

Here we presented for brevity the explicit expression for a part of Hamiltonian (5) only without the last term. Using (17) - (19) we find the Dyson equation in the Wannier basis

$$G^{\mu\nu}(ij; \omega) = G_0^{\mu\nu}(ij; \omega) + \sum_{m n \alpha \beta} G_0^{\mu\alpha}(im; \omega) M^{\alpha\beta}(mn; \omega) G^{\beta\nu}(nj; \omega) \quad (41)$$

The equation (41) is the central result of the present treatment.

7 Quasiparticle Formulation

Let us first consider how to describe our system in terms of quasiparticles. For a translationally invariant system, to describe the low-lying excitations in terms of quasiparticles one has to make a Fourier transformation

$$\begin{aligned} G^{\mu\nu}(ij; \omega) &= N^{-1} \sum_k \exp[ik(R_i - R_j)] G^{\mu\nu}(k; \omega) \\ M^{\mu\nu}(ij; \omega) &= N^{-1} \sum_k \exp[ik(R_i - R_j)] M^{\mu\nu}(k; \omega) \\ t_{ij}^{\mu\mu} &= N^{-1} \sum_k \exp[ik(R_i - R_j)] \epsilon_\mu(k) \end{aligned} \quad (42)$$

The Dyson equation (41) in the Bloch vector space is given by

$$G^{\mu\nu}(k; \omega) = G_0^{\mu\nu}(k; \omega) + \sum_{\alpha\beta} G_0^{\mu\alpha}(k; \omega) M^{\alpha\beta}(k; \omega) G^{\beta\nu}(k; \omega) \quad (43)$$

The renormalized energies in the mean field approximations are the solutions of the equation

$$\sum_{\alpha} F^{\mu\alpha}(k) G_0^{\alpha\nu}(k; \omega) = 1 \delta_{\mu\nu} \quad (44)$$

Using (44) we find

$$E_{11}^{\alpha\nu}(k) = [\omega - \epsilon_\alpha(k)]\delta_{\alpha\nu} - (1 - \delta_{\alpha\nu})(V - I)K_{\uparrow\uparrow}^{\alpha\nu} - \sum_\mu [(1 - \delta_{\alpha\mu})\delta_{\alpha\nu}(V - I)N_\uparrow^\mu + (U\delta_{\alpha\mu} + V(1 - \delta_{\alpha\mu}))\delta_{\alpha\nu}N_\downarrow^\mu]; \quad (45)$$

$$E_{12}^{\alpha\nu}(k) = [U\delta_{\alpha\nu} + V(1 - \delta_{\alpha\nu})]K_{\uparrow\downarrow}^{\alpha\nu}; \quad (46)$$

$$N_\sigma^\alpha = N^{-1} \sum_p \langle a_{p\alpha\sigma}^+ a_{p\alpha\sigma} \rangle; \quad (47)$$

$$K_{\sigma_1\sigma_2}^{\alpha\beta} = N^{-1} \sum_p \langle a_{p\alpha\sigma_1} a_{p\beta\sigma_2}^+ \rangle \quad (48)$$

For the degenerate Hubbard model ($V = I = J = 0$) we get

$$E_{11}^{\alpha\nu}(k) = [\omega - \epsilon_\alpha(k) - UN_\downarrow^\alpha]\delta_{\alpha\nu} \quad (49)$$

The spectrum of electronic low-lying excitations without damping follows from the poles of the single-particle mean-field GF

$$\begin{pmatrix} \hat{E}_{11} & \hat{E}_{12} \\ \hat{E}_{21} & \hat{E}_{22} \end{pmatrix} \begin{pmatrix} \hat{G}_{011} & \hat{G}_{012} \\ \hat{G}_{021} & \hat{G}_{022} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (50)$$

Here \hat{G}_0 denotes a matrix in the space of band indices. If we put the spin-flip contributions equal to zero, i.e.

$$\hat{E}_{12} = \hat{E}_{21} = 0$$

then the quasiparticle spectra are given by

$$\det|\hat{E}_{11}| = 0; \quad \det|\hat{E}_{22}| = 0$$

For the multiorbital Hubbard model (5) we find

$$G_{011}^\alpha(\omega) = [\omega - \epsilon_\alpha(k) - UN_\downarrow^\alpha - V \sum_\nu (1 - \delta_{\alpha\nu})(N_\downarrow^\nu + N_\uparrow^\nu) + I \sum_\nu (1 - \delta_{\alpha\nu})N_\uparrow^\nu]^{-1} \quad (51)$$

Finally we turn to the calculation of the damping. To find the damping of the electronic states in the general case, one needs to find the matrix elements of the self-energy in (43). Thus we have

$$\begin{pmatrix} \hat{G}_{11} & \hat{G}_{12} \\ \hat{G}_{21} & \hat{G}_{22} \end{pmatrix} = \left[\begin{pmatrix} \hat{G}_{011} & \hat{G}_{012} \\ \hat{G}_{021} & \hat{G}_{022} \end{pmatrix}^{-1} - \begin{pmatrix} \hat{M}_{11} & \hat{M}_{12} \\ \hat{M}_{21} & \hat{M}_{22} \end{pmatrix} \right]^{-1} \quad (52)$$

From this matrix equation we have

$$\begin{aligned} \hat{G}_{11} &= (\hat{G}_{011}^{-1} - \hat{\Sigma}_{11})^{-1}; & \hat{G}_{21} &= (\hat{G}_{021}^{-1} - \hat{\Sigma}_{21})^{-1}; \\ \hat{G}_{12} &= (\hat{G}_{012}^{-1} - \hat{\Sigma}_{12})^{-1}; & \hat{G}_{22} &= (\hat{G}_{022}^{-1} - \hat{\Sigma}_{22})^{-1}; \end{aligned} \quad (53)$$

where the true self-energy has the form

$$\hat{\Sigma}_{11} = \hat{M}_{11} - \hat{E}_{12}\hat{E}_{22}^{-1}\hat{M}_{21} + \left[\hat{M}_{12}\hat{E}_{22}^{-1} + (\hat{M}_{12} - \hat{E}_{12})\hat{E}_{22}^{-1}\hat{M}_{22}(\hat{E}_{22} - \hat{M}_{22})^{-1} \right] (\hat{M}_{21} - \hat{E}_{21}) \quad (54)$$

The elements of the mass operator matrix \hat{M} are proportional to the higher-order GF of the following form

$$(^{(ir)}) \langle \langle a_{k+p\alpha\sigma_1} a_{p+q\nu\sigma_2}^+ a_{q\nu\sigma_2} | a_{k+s\beta\sigma_3}^+ a_{r\mu\sigma_4}^+ a_{r+s\mu\sigma_4} \rangle \rangle^{(ir),p}$$

For the explicit approximate calculation of the elements of the self-energy it is convenient to write down the GFs in (54) in terms of correlation functions by using the well-known spectral theorem [53]:

$$\begin{aligned} (^{(ir)}) \langle \langle a_{k+p\alpha\sigma_1} a_{p+q\nu\sigma_2}^+ a_{q\nu\sigma_2} | a_{k+s\beta\sigma_3}^+ a_{r\mu\sigma_4}^+ a_{r+s\mu\sigma_4} \rangle \rangle^{(ir),p} = \\ \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'} (\exp(\beta\omega') + 1) \int_{-\infty}^{+\infty} \exp(-i\omega't) dt \\ \langle a_{k+s\beta\sigma_3}^+(t) a_{r\mu\sigma_4}^+(t) a_{r+s\mu\sigma_4}(t) | a_{k+p\alpha\sigma_1} a_{p+q\nu\sigma_2}^+ a_{q\nu\sigma_2} \rangle^{(ir),p} \end{aligned} \quad (55)$$

Further insight is gained if we select the suitable relevant “trial” approximation for the correlation function on the r.h.s. of (55). In this paper we show that the earlier formulations, based on the decoupling or/and on diagrammatic methods can be arrived at from our technique but in a self-consistent way. Clearly the choice of the relevant trial approximation for the correlation function in (55) can be done in a few ways. For example, a reasonable and workable one may be the following “pair approximation” [3], which is especially suitable for low density of the quasiparticles:

$$\begin{aligned} & \langle a_{k+s\beta\sigma}^+(t) a_{r\mu-\sigma}^+(t) a_{r+s\mu-\sigma}(t) a_{k+p\alpha\sigma} a_{p+q\nu-\sigma}^+ a_{q\nu-\sigma} \rangle^{ir} \approx \\ & \langle a_{k+s\beta\sigma}^+(t) a_{k+p\alpha\sigma} \rangle \langle a_{r\mu-\sigma}^+(t) a_{q\nu-\sigma} \rangle \langle a_{r+s\mu-\sigma}(t) a_{p+q\nu-\sigma}^+ \rangle \\ & + \langle a_{k+s\beta\sigma}^+(t) a_{q\nu-\sigma} \rangle \langle a_{r\mu-\sigma}^+(t) a_{k+p\alpha\sigma} \rangle \langle a_{r+s\mu-\sigma}(t) a_{p+q\nu-\sigma}^+ \rangle \end{aligned} \quad (56)$$

Using (56) in (55) we obtain the approximate expression for the self-energy operator in a self-consistent form (the self-consistency means that we express approximately the self-energy operator in terms of the initial GF and, in principle, one can obtain the required solution by a suitable iteration procedure):

$$\begin{aligned} M_{11}^{\alpha\beta}(k, \omega) = \frac{1}{N^2\pi^3} \sum_{pq\mu\nu} (B_1^{\alpha\nu} B_1^{\mu\beta} \int \frac{d\omega_1 d\omega_2 d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} \\ N(\omega_1, \omega_2, \omega_3) [g_{p+q\uparrow\uparrow}^{\mu\nu}(\omega_1) g_{q\uparrow\uparrow}^{\nu\mu}(\omega_2) g_{k+p\uparrow\uparrow}^{\alpha\beta}(\omega_3) + g_{k+p\uparrow\uparrow}^{\alpha\mu}(\omega_3) g_{q\uparrow\uparrow}^{\nu\beta}(\omega_2) g_{p+q\uparrow\uparrow}^{\mu\nu}(\omega_1)] + \\ B_1^{\alpha\nu} B_2^{\mu\beta} \int \frac{d\omega_1 d\omega_2 d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} N(\omega_1, \omega_2, \omega_3) [(\downarrow\uparrow)(\uparrow\downarrow)(\uparrow\uparrow) + (\uparrow\downarrow)(\downarrow\uparrow)(\uparrow\uparrow)] + \\ B_2^{\alpha\nu} B_1^{\mu\beta} \int \frac{d\omega_1 d\omega_2 d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} N(\omega_1, \omega_2, \omega_3) [(\uparrow\downarrow)(\downarrow\uparrow)(\uparrow\uparrow) + (\uparrow\uparrow)(\uparrow\downarrow)(\downarrow\uparrow)] + \\ B_2^{\alpha\nu} B_2^{\mu\beta} \int \frac{d\omega_1 d\omega_2 d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} N(\omega_1, \omega_2, \omega_3) [(\downarrow\downarrow)(\downarrow\downarrow)(\uparrow\uparrow) + (\uparrow\downarrow)(\downarrow\downarrow)(\uparrow\uparrow)] \end{aligned} \quad (57)$$

where we have used the notations

$$N(\omega_1, \omega_2, \omega_3) = [n(\omega_2)n(\omega_3) + n(\omega_1)(1 - n(\omega_2) - n(\omega_3))];$$

$$g_{k\sigma\sigma'}(\omega) = -\frac{1}{\pi} \text{Im}G_{k\sigma\sigma'}(\omega + i\varepsilon); \quad n(\omega) = [\exp(\beta\omega) + 1]^{-1}$$

Here we present for brevity the explicit expression for a part of the Hamiltonian only without the last term. The equations (43) and (57) form a closed self-consistent system of equations for the single-electron GF for the Hubbard model, but for the weakly correlated limit only. In principle, one may use on the r.h.s. of (57) any workable first iteration-step forms of the GFs and find a solution by repeated iterations. It is most convenient to choose as the first iteration step the following simple one-pole approximation:

$$g_{k\sigma}(\omega) \approx \delta(\omega - \epsilon(k\sigma)) \quad (58)$$

Then, using (58) in (57), one can get an explicit expression for the self-energy. However, the actual explicit calculations will be much more transparent if we confine ourselves to the single-orbital Hubbard model in order to discuss more explicitly the reliability of the present approach.

8 Antiferromagnetic Single-Particle States

The technique for obtaining of the antiferromagnetic solutions to the correlated fermions on a lattice is presented in this section for the single-orbital Hubbard model (10). In general, it can be easily applied for the multiorbital extended Hubbard model.

As discussed above, the self-consistent approach to the calculation of the one-particle properties requires the calculation of the following GF

$$\begin{pmatrix} \langle\langle a_{i\sigma} | a_{j\sigma}^+ \rangle\rangle & \langle\langle a_{i\sigma} | a_{j-\sigma}^+ \rangle\rangle \\ \langle\langle a_{i-\sigma} | a_{j\sigma}^+ \rangle\rangle & \langle\langle a_{i-\sigma} | a_{j-\sigma}^+ \rangle\rangle \end{pmatrix} = \hat{G}(ij; \omega) \quad (59)$$

The equation of motion for the Fourier transform of the GF has the form

$$\sum_m \hat{A}(im) \hat{G}(mj; \omega) = \delta_{ij} \delta_{\sigma\sigma'} + U \langle\langle a_{i\sigma} n_{i-\sigma} | a_{j\sigma'}^+ \rangle\rangle \quad (60)$$

where

$$\hat{A}(im) = \begin{pmatrix} (\omega\delta_{mi} - t_{im}) & 0 \\ 0 & (\omega\delta_{mi} - t_{im}) \end{pmatrix} \quad (61)$$

Using the definition of the irreducible parts (26) the equation of motion can be exactly transformed to the following form

$$\sum_m \hat{A}_1(im) \hat{G}(mj; \omega) = \delta_{ij} \delta_{\sigma\sigma'} + U \hat{D}^{ir}(ij; \omega) \quad (62)$$

where

$$\hat{A}_1(im) = \begin{pmatrix} (\omega\delta_{mi} - t_{im} - U \langle n_{i-\sigma} \rangle) & -U \langle a_{i\sigma} a_{i-\sigma}^+ \rangle \\ -U \langle a_{i-\sigma} a_{i\sigma}^+ \rangle & (\omega\delta_{mi} - t_{im} - U \langle n_{i\sigma} \rangle) \end{pmatrix} \quad (63)$$

To calculate the irreducible higher-order GF D^{ir} we have to write the equation of motion for it. After introducing the irreducible parts for the operators in the right-hand-side we find

$$\sum_n \hat{D}^{ir}(in; \omega) \hat{A}_2(nj) = U^2 \hat{D}_1(ij; \omega) \quad (64)$$

where

$$\hat{D}_1(ij; \omega) = \begin{pmatrix} ^{(ir)} \langle\langle a_{i\sigma} n_{i-\sigma} | a_{j\sigma}^+ n_{j-\sigma} \rangle\rangle ^{(ir)} & ^{(ir)} \langle\langle a_{i\sigma} n_{i-\sigma} | a_{j-\sigma}^+ n_{j\sigma} \rangle\rangle ^{(ir)} \\ ^{(ir)} \langle\langle a_{i-\sigma} n_{i\sigma} | a_{j\sigma}^+ n_{j-\sigma} \rangle\rangle ^{(ir)} & ^{(ir)} \langle\langle a_{i-\sigma} n_{i\sigma} | a_{j-\sigma}^+ n_{j\sigma} \rangle\rangle ^{(ir)} \end{pmatrix} \quad (65)$$

Then equation of motion for the GF can be exactly transformed into the following scattering equation

$$G(ij; \omega) = G_0(ij; \omega) + \sum_{mn} G_0(im; \omega) P(mn; \omega) G_0(nj; \omega) \quad (66)$$

where the generalized mean-field GF G_0 reads

$$\sum_m A_1(im) G_0(mj; \omega) = \delta_{ij} \quad (67)$$

and the scattering operator P has the form

$$\hat{P}(ij; \omega) = U^2 \begin{pmatrix} \langle \langle a_{i\sigma} n_{i-\sigma} | a_{j\sigma}^+ n_{j-\sigma} \rangle \rangle^{(ir)} & \langle \langle a_{i\sigma} n_{i-\sigma} | a_{j-\sigma}^+ n_{j\sigma} \rangle \rangle^{(ir)} \\ \langle \langle a_{i-\sigma} n_{i\sigma} | a_{j\sigma}^+ n_{j-\sigma} \rangle \rangle^{(ir)} & \langle \langle a_{i-\sigma} n_{i\sigma} | a_{j-\sigma}^+ n_{j\sigma} \rangle \rangle^{(ir)} \end{pmatrix} \quad (68)$$

The Dyson equation (41) then will be reduced for the single-band Hubbard model to the following form

$$G(ij; \omega) = G_0(ij; \omega) + \sum_{mn} G_0(im; \omega) M(mn; \omega) G(nj; \omega) \quad (69)$$

The mass operator $M(mn; \omega) = U^2 P^{(p)}(mn; \omega)$ describes the inelastic (retarded) part of the electron-electron interaction. For the purpose of analogy with the theory of superconductivity [19] let us write the Hartree-Fock (elastic) part of the Coulomb mass operator (not included in (68)):

$$\hat{M}^{HF}(im) = U \begin{pmatrix} \langle n_{i-\sigma} \rangle & \langle a_{i\sigma} a_{i-\sigma}^+ \rangle \\ \langle a_{i-\sigma} a_{i\sigma}^+ \rangle & \langle n_{i\sigma} \rangle \end{pmatrix} \delta_{im} \quad (70)$$

To obtain workable expressions for various parts of the mass operator we use the spectral theorem, inverse Fourier transformation and make relevant approximation in the time correlation functions. In analogy with the theory of superconductivity the suitable approximation which describe the interaction between the charge and spin collective excitations can be written as

$$\begin{aligned} & \langle a_{n\sigma}^+(t) a_{n-\sigma}^+(t) a_{n-\sigma}(t) a_{m\sigma} a_{m-\sigma}^+ a_{m-\sigma} \rangle^{ir} \approx \\ & \quad \langle a_{n\sigma}^+(t) a_{m\sigma} \rangle \langle n_{n-\sigma}(t) n_{m-\sigma} \rangle \\ & + \langle a_{n-\sigma}^+(t) a_{m-\sigma} \rangle \langle a_{n\sigma}^+(t) a_{n-\sigma}(t) a_{m\sigma} a_{m-\sigma}^+ \rangle \\ & + \langle a_{n-\sigma}(t) a_{m-\sigma}^+ \rangle \langle a_{n\sigma}^+(t) a_{n-\sigma}(t) a_{m\sigma} a_{m-\sigma} \rangle \\ & + \langle a_{n\sigma}^+(t) a_{m-\sigma} \rangle \langle a_{n-\sigma}^+(t) a_{n-\sigma}(t) a_{m\sigma} a_{m-\sigma}^+ \rangle \\ & + \langle a_{n-\sigma}^+(t) a_{m\sigma} \rangle \langle a_{n\sigma}^+(t) a_{n-\sigma}(t) a_{m-\sigma}^+ a_{m-\sigma} \rangle \\ & + \langle a_{m-\sigma}(t) a_{m\sigma} \rangle \langle a_{n\sigma}^+(t) a_{n-\sigma}(t) a_{m-\sigma}^+ a_{m-\sigma} \rangle \end{aligned} \quad (71)$$

The suitable or relevant approximations follow from the concrete physical conditions of the problem under consideration. We consider here for illustration the contributions from charge and spin collective degrees of freedom. We get

$$\begin{aligned} M(ij; \omega) = & \frac{U^2}{2\pi^2} \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{ctg \frac{\beta\omega_1}{2} + tg \frac{\beta\omega_2}{2}}{\omega - \omega_1 - \omega_2} \\ & \left(\begin{pmatrix} Im \langle \langle n_{i-\sigma} | n_{j-\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i\sigma} | a_{j\sigma}^+ \rangle \rangle_{\omega_2} & Im \langle \langle n_{i-\sigma} | n_{j\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i\sigma} | a_{j-\sigma}^+ \rangle \rangle_{\omega_2} \\ Im \langle \langle n_{i\sigma} | n_{j-\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i-\sigma} | a_{j\sigma}^+ \rangle \rangle_{\omega_2} & Im \langle \langle n_{i\sigma} | n_{j\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i-\sigma} | a_{j-\sigma}^+ \rangle \rangle_{\omega_2} \end{pmatrix} + \right. \\ & \left. \begin{pmatrix} Im \langle \langle S_i^{-\sigma} | S_j^{\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i-\sigma} | a_{j-\sigma}^+ \rangle \rangle_{\omega_2} & Im \langle \langle S_i^{-\sigma} | S_j^{-\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i-\sigma} | a_{j\sigma}^+ \rangle \rangle_{\omega_2} \\ Im \langle \langle S_i^{\sigma} | S_j^{\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i\sigma} | a_{j-\sigma}^+ \rangle \rangle_{\omega_2} & Im \langle \langle S_i^{\sigma} | S_j^{-\sigma} \rangle \rangle_{\omega_1} & Im \langle \langle a_{i\sigma} | a_{j\sigma}^+ \rangle \rangle_{\omega_2} \end{pmatrix} \right) \end{aligned} \quad (72)$$

It shows that it is possible to do all calculations in the localized Wannier basis as we did in deriving the equations for the strong coupling superconductivity in transition metals [19]. This has great advantage for consideration of disordered transition metal alloys.

As for the translationally invariant crystal with broken symmetry the following special Fourier transform should be performed for the generalized mean-field GF $G_0(ij; \omega)$ (67)

$$\begin{aligned} G_0^{11}(ij; \omega) &= \sum_k \exp[ik(R_i - R_j)] G_0^{11}(k; \omega) \\ G_0^{12}(ij; \omega) &= \sum_k \exp[ikR_i - i(k+Q)R_j] G_0^{12}(k; \omega) \\ G_0^{21}(ij; \omega) &= \sum_k \exp[i(k+Q)R_i - ikR_j] G_0^{21}(k; \omega) \\ G_0^{22}(ij; \omega) &= \sum_k \exp[i(k+Q)(R_i - R_j)] G_0^{22}(k; \omega) \end{aligned} \quad (73)$$

The result of this transformation is then

$$G_0 = \begin{pmatrix} G_0^{11} & G_0^{12} \\ G_0^{21} & G_0^{22} \end{pmatrix} = \frac{\begin{pmatrix} \omega - E_{\downarrow}^{HF}(k+Q) & \Delta_{\uparrow\downarrow}(k) \\ \Delta_{\downarrow\uparrow}(k) & \omega - E_{\uparrow}^{HF}(k) \end{pmatrix}}{(\omega - E_1^{MF}(k))(\omega - E_2^{MF}(k))} \quad (74)$$

where

$$\begin{aligned} E_{\sigma}^{HF} &= \epsilon(k) + U < n_{\sigma} > \\ \Delta_{\sigma-\sigma}(k) &= U \sum_i i \exp(ikR_i) < a_{i\sigma} a_{i-\sigma}^+ > \\ E_{1,2}^{MF} &= \left(\frac{E_{\uparrow}^{HF}(k) + E_{\downarrow}^{HF}(k+Q)}{2} \pm \sqrt{\left(\frac{E_{\uparrow}^{HF}(k) - E_{\downarrow}^{HF}(k+Q)}{2} \right)^2 + \Delta_{\uparrow\downarrow}(k)\Delta_{\downarrow\uparrow}(k)} \right) \end{aligned} \quad (75)$$

It is evident that one can define the Overhauser's angle θ_k

$$\cos^2 \theta_k = \frac{\Delta_{\uparrow\downarrow}(k)\Delta_{\downarrow\uparrow}(k)}{(\omega - E_{\uparrow}^{HF}(k))^2 + \Delta_{\uparrow\downarrow}(k)\Delta_{\downarrow\uparrow}(k)} \quad (76)$$

In Overhauser's notations $\Delta_{\uparrow\downarrow}(k) = \Delta_{\downarrow\uparrow}(k) = \Delta$. The self-consistent set of equations for determining of the SDW (or "gap") order parameter Δ , chemical potential μ and averaged moment $< s^z >$ is

$$\begin{aligned} \Delta &= U/N \sum_k < a_{k+Q\downarrow}^+ a_{k\uparrow} > \\ < s^z > &= U/N \sum_k < a_{k\uparrow}^+ a_{k\uparrow} - a_{k\downarrow}^+ a_{k\downarrow} > \\ n &= N^{-1} \sum_k (n(E_1^{MF}(k)) + n(E_2^{MF}(k))) \end{aligned} \quad (77)$$

The above expressions were derived for correlated itinerant fermions on a lattice within the Hubbard model and for finite temperatures. These equations were also deduced in previous papers in the course of their analysis. Here we deduced it by using more sophisticated arguments of the IGFs method in complete analogy with our description of the Heisenberg antiferromagnet

at finite temperatures [52]. However, the self-consistent system of equations (69), (72) for determining the quasiparticle spectra with damping is not as obvious as generalization as the equations (77). This is intrinsically the many-body manifestation of the correlation effects of itinerant fermions on a lattice and shows clearly the advantage of the present approach.

To confirm this, the explicit calculation of the damping should be performed. The natural way to tackle this program would then to look at the calculations of the collective GFs of the generalized spin (and charge) susceptibilities in (72) but this deserves of separate consideration. Again this problem bears close similarity to the paramagnetic Hubbard model and the antiferromagnetic Heisenberg model and it can be argued that this effect of interference of single-particle and collective modes of excitations should be considered carefully.

9 Discussion

We have been concerned in this paper with establishing the essence of single-particle excitations of correlated lattice fermions, rather than with their detailed properties. We have considered the single- and multiband Hubbard model but the calculational details were mainly presented for the single-band Hubbard model where the appropriate concepts are easier to demonstrate. We have considered a general family of symmetry broken solutions for itinerant lattice fermions, identifying the type of ordered states and then derived explicitly the functional of generalized mean fields and the self-consistent set of equations which describe the quasiparticle spectra and their damping in the most general way. While such generality is not so obvious in all applications, it is highly desirable in treatments of such complicated problems as the competition and interplay of antiferromagnetism and superconductivity, heavy fermions and antiferromagnetism etc., because of the non-trivial character of coupled equations which occur there. Both these problems are subject of current but independent research.

Another development of the present approach is the consideration of the itinerant antiferromagnetism of highly correlated lattice fermions when U is very large but finite. Like the weakly-coupled case described in this paper, the symmetry broken approach will work, but matters are complicated by the necessity of constructing the more extended algebra of relevant operators [3]. This idea has been carried out for the paramagnetic solution of the single-band Hubbard model [10]. It would be interesting to understand on a deeper level the relationship between Mott-Hubbard metal-insulator transition and various ordered magnetic states within the Hubbard model.

In conclusion, we have demonstrated that the Irreducible Green's Functions approach is a workable and efficient scheme for the consistent description of the correlated fermions on a lattice at finite temperatures and that it can be generalized naturally to include the symmetry broken concept.

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